Ethyl hydroperoxide

3031-74-1 | DTXSID70184402

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.02 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.63e-01

Confidence level: 5.66e-01

Nearest Neighbors from the Training Set

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Methanesulfonic acid
Measured: 5.47
Predicted: 1.37e-03

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N-Methylethanolamine
Measured: 9.50
Predicted: 3.60e-01

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1,4-Dichlorobutane
Measured: 5.31
Predicted: 6.71

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Trichloroethylene
Measured: 14.5
Predicted: 94.3